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ADSORPTION CHARACTERIZATION OF COMPOSITE ACTIVATED CARBON FOR APPLICATION IN ADSORPTION COOLING SYSTEMS

ABSTRACT

for the dissertation work of Berdenova B.A., for the degree of Doctor of Philosophy (PhD) in the specialty “6D060300 – Mechanics”.

Relevance of the research topic. According to International Institute of Refrigeration (IIR), approximately 15% of all electricity produced worldwide is used for refrigeration and air conditioning, which means the huge portion of the energy consumed falls to the share of different cooling systems. While using an adsorption process for cooling applications, the electrically powered compressors of conventional compression based systems replaced by thermally driven adsorption bed. This makes ACS fully functional without electricity supply, which allows the use of this technology in remote undeveloped regions. Development of such technology would be useful for Kazakhstan where the towns and villages are very scattered throughout the country. Introduction of the fully solar driven adsorption cooling systems would have a positive socio-economic effect via rational use of energy and its safe operation. The transition to the clean sources of energy would solve different problems with air pollution.

The scientific direction of the research is almost new and developing slowly in Kazakhstan, therefore there are no specialized laboratories equipped with the necessary equipment for developing new types of adsorbents for refrigeration systems, and for analyzing their physical properties. Whereas around the world the given field actively developing. Therefore the research topic is very important and significant on a national scale.

Moreover, the adsorption process is finding application in various fields of science when creating new technologies and techniques. For instances: gas storage, heat pumps, CO_2 capture and sequestration, etc. Therefore new adsorbents with improved characteristics are being developed and proposed by different authors. An accurate assessment of the adsorption characteristics of newly synthesized materials plays a very important role in determining their thermodynamic properties and forecasting their performance as they used in different systems. Therefore the results of the study also can be used in other adsorption related systems.

Purpose of the study. To determine physical and adsorption properties of the newly synthesized composite activated carbon and develop a scientific basis for the selection of materials for adsorption cooling systems using experimental and numerical methods.

The objectives of the study.

- to conduct experiments to measure the thermal and porous properties of the composite activated carbon;

- to determine adsorption characteristics of carbon dioxide onto the composite material for possible applications in adsorption cooling systems;
- to investigate regularities of isothermal adsorption process using numerical method and determine dynamic characteristics of the process of adsorption.

Object of the research. Composite activated carbon, carbon dioxide adsorption onto consolidated activated carbon, adsorption cooling systems.

Subject of the research. Thermal and adsorption characteristics of composite activated carbon.

Methods. Experimental, mathematical and numerical modeling. Experiments were held at I2CNER Institute in conjunction with the lab members. To analyze the experimental data different regression and other known analytical methods were used. Sample of consolidated activated carbon for study was provided by I2CNER.

The scientific novelty of the study.

- New composite adsorbent with enhanced thermal conductivity and adsorption capacity was synthesized and analyzed comprehensively: the developed consolidated adsorbent demonstrated 233% higher thermal conductivity than that of parent adsorbent;
- Absolute uptake was estimated from excess adsorption in two steps, which allowed more accurate estimation, and adsorption isotherm models constructed. Results indicated good approximation between data points and model. Correlation errors RMSD for modified D-A and Tóth models were 0.62% and 0.56% respectively;
- New mathematical model considering the adsorption caused porosity and Knudsen diffusivity changes was developed. The temperature dependent adsorption rate change due to the energy release during adsorption process is also implemented in the model. The effective Knudsen diffusion coefficient for the working pair of CO_2/AC evaluated from Pore Size Distribution data. The experiment conducted on the magnetic suspension balance unit (MSB-GS-100-10 M) to measure the CO_2 adsorption onto composite activated carbon was simulated.

Validity and reliability. The validity and reliability of the scientific conclusions obtained in the thesis are confirmed by their consistent theoretical and mathematical justification, as well as obtained simulation results compared with experimental data.

Theoretical and practical significance. Theoretical significance is that the developed mathematical model predicts the adsorption dynamics with better accuracy as it takes into account such factors like porosity and permeability changes with uptake, and adsorption rate changes due to temperature variations as the process of adsorption is exothermic.

The research has a practical significance, because the enhancement of adsorption characteristics of the working pair (refrigerant/adsorbent) in ACS has a positive impact on its performance. Results obtained later will be used in development of the fully solar driven ACS prototype. Such technology could be used in production of from small thermostats till huge storehouses with regulated temperature.

Testing the results of the study. The results obtained on the topic of the work were presented at the following scientific events:

- Report at the city scientific seminar “Mathematical problems of natural science. Inverse and incorrect tasks”, Almaty, 2019;
- International scientific conference of students and young scientists “FARABI ALEMI”, Almaty, April 8-11, 2019;
- International scientific conference of students and young scientists "FARABI ALEMI", Almaty, April 10-12, 2018;
- XIII International Scientific Conference of Students, Undergraduates and Young Scientists "Lomonosov-2017", Astana, April 14-15, 2017.

Series of presentations given at the “Fluid mechanics” scientific seminars and the meeting of the department of “Mechanics”. The results of the research were published in scientific journals: 3 publications in journals recommended by the Committee on the Control of Education and Science of the RK and 1 publication in international peer-reviewed journal *International Journal of Refrigeration* with an impact factor of 3.2 indexed in Scopus DB.

The reliability and validity of the scientific provisions, conclusions and results of the dissertation is confirmed by the publication of the results in journal having non-zero impact factor.

Assessment of the completeness of the objectives of the study.

All the research objectives are fulfilled. The dissertation is a complete independent research work devoted to the study of the thermal and adsorption characteristics of consolidated activated carbon for use in adsorption cooling systems. The results of the study and the obtained dependence curves are relevant.

Provisions to be defended.

- New composite adsorbent with enhanced thermal conductivity and adsorption capacity was synthesized and analyzed comprehensively: the developed consolidated adsorbent demonstrated 233% higher thermal conductivity than that of parent adsorbent;
- Absolute uptake was estimated from excess adsorption in two steps, which allowed more accurate estimation, and adsorption isotherm models constructed. Results indicated good approximation between data points and model. Correlation errors RMSD for modified D-A and Tóth models were 0.62% and 0.56% respectively;
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Scientific internships. International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University, Fukuoka, Japan, June-July 2017.

Publications. The results of the research were discussed and reported at conferences, and published in scientific journals: 3 publications in journals

recommended by the Committee on the Control of Education and Science of the RK and 1 publication in international peer-reviewed journal *International Journal of Refrigeration* with an impact factor of 3.2 indexed in Scopus DB. The results on the topic of the dissertation were published in the following papers:

Publications in journals:

1) B.Berdenova and A.Kaltayev, "Review of adsorption and thermal characteristics of activated carbon and its application in ANG storage and ACS systems", Vestnik nacional'noj akademii nauk RK, Kazakhstan, 2017, #3, Pages 27-36.
2) B.Berdenova, Ye.Maksum, "Regressionnyj analiz dlja opredelenija parametrov modelej izoterm adsorbcii", Vestnik KazNITU, 2018, #4, Pages 233-240.
3) B. Berdenova, A. Pal, M. Muttakin, S. Mitra, K. Thu, B.B. Saha, A. Kaltayev, "A comprehensive study to evaluate absolute uptake of carbon dioxide adsorption onto composite adsorbent", International Journal of Refrigeration, Volume 100, April 2019, Pages 131-140, **Scopus** (IF 3.17), https://doi.org/10.1016/j.ijrefrig.2019.01.014
4) B.Berdenova, "Matematicheskaja model' processa dokriticheskoj izotermicheskoj adsorbcii CO_2 na aktivirovannyj ugol'", Vestnik KazNITU, 2019, #6, Pages 751-756.

Abstracts in conference proceedings:

1) B. Berdenova, thesis in conference proceeding "Stacionarnye sistemy adsorbcionnogo ohlazhdenija, rabotajushhie na jekologicheski chistyh hladagentah", "XIII Mezhdunarodnaja nauchnaja konferencija studentov, magistrantov i molodyh uchenyh "Lomonosov – 2017", Kazahstani brunch of Moscow State University named after M.V. Lomonosov, Astana, 2017.
2) Ye. Maksum, B. Berdenova, thesis in conference proceeding "Termodinamicheskij analiz adsorbcionnoj sistemy ohlazhdenija s rabochej paroj aktivirovannyj ugol'/CO_2, «V Mezhdunarodnye Farabievskie chtenija», Almaty, 2018.
3) B. Berdenova, "Sverhkriticheskij tsikl raboty holodil'nogo oborudovanija na uglekislom gaze", "Mezhdunarodnye Farabievskie chtenija", Almaty, 2019.

Structure and scope of the Ph.D. thesis. The text of the thesis contains the following elements: abstract, introduction, 5 chapters, conclusion, the reference list of 67 items and the list of publication on the topic of the Ph.D. thesis 7 items. The work has been expounded in 65 pages, contains 30 figures and 8 tables. Chapters 3-6 are done in collaboration with the foreign supervisor's group and done as part of a scientific internship to Japan. On collaboration results the joint paper was published.

The introduction of the dissertation provides an overview of adsorption cooling systems, the principle of operation of such systems, advantages and disadvantages. It also lists the main methods for increasing the cooling capacity of the material, and ways to make adsorption reactors more compact. The main methods used are the consolidation and enhancement in thermal conductivity of the activated carbon.

The third chapter describes the method and operating principle of an experimental setup for measuring absorption uptake for a working pair of activated carbon/carbon dioxide. Other established intrinsic and adsorption characteristics of the composite material are also listed.

In the fourth and fifth chapters the methods for estimating the absolute uptake using two different assumptions and correlation of the parameters of the Dubinin-Astakhov and Toss isotherm models are described. In the sixth chapter the isosteric heat of adsorption is studied.

In the seventh chapter, the effective Knudsen diffusion coefficient for a porous medium is obtained using the pore size distribution and the characteristics of the defunding gas.

To calculate the adsorption uptake at the solid-gas interface, and for a detailed description of the dynamics of the adsorption process, a mathematical model of the non-isothermal reactive adsorption was constructed and solved. The mathematical model considers the adsorption caused porosity and Knudsen diffusivity changes. The experiment conducted on the magnetic suspension balance unit (MSB-GS-100-10 M) to measure the CO_2 adsorption onto composite activated carbon was simulated.

The result obtained was compared with the results found using non-reactive isothermal model and experimental data. Non-isothermal reactive flow model gives more accurate curve of volume averaged uptake with sharp increase in the adsorption starting and lower rate of mass uptake due to the release of the heat of adsorption. The rate gradually increases with time as the thermal energy dissipates to the surrounding through natural convection. Thus, the dependence curves obtained by this method show better agreement with the experimental results. Residual deviations/errors in the results are associated with the use of 1D model assumption that excludes the gas penetration by the sides of the tablet.

In conclusion, the main results and conclusions of the thesis are presented. Comparison with experimental data shows good measurement accuracy. The results of the presented dissertation are of great theoretical significance, and can be used for a detailed description of the dynamics of adsorption of carbon dioxide in consolidated activated carbon. The main provisions and conclusions of the dissertation are justified.